

FINITE-SIZE SCALING AND POWER LAW RELATIONS FOR DIPOL-QUADRUPOLE INTERACTION ON BLUME-EMERY-GRIFFITHS MODEL

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Abstract: The Blume-Emery-Griffiths model with the dipol-quadrupol interaction (ℓ) has been simulated using a cellular automaton algorithm improved from the Creutz cellular automaton (CCA) on the face centered cubic (fcc) lattice. The finite-size scaling relations and the power laws of the order parameter (M) and the susceptibility (χ) are proposed for the dipol-quadrupol interaction (ℓ). The dipol-quadrupol critical exponent δ_ℓ has been estimated from the data of the order parameter (M) and the susceptibility (χ). The simulations have been done in the interval $0 \leq \ell = L/J \leq 0.01$ for $d = D/J = 0$, $k = K/J = 0$ and $h = H/J = 0$ parameter values on a face centered cubic (fcc) lattice with periodic boundary conditions. The results indicates that the effect of the ℓ parameter is similar to the external

magnetic field (h). The critical exponent δ_ℓ are in good agreement with the universal value ($\delta_h = 5$) of the external magnetic field.

Keywords: Cellular automaton, face-centered cubic, Blume-Emery-Griffiths model, critical exponent

The spin-1 Ising model, which is known as the generalized Blume-Emery-Griffiths (BEG) model, can be used to simulate many physical systems. The model firstly has been presented for describing phase separation and superfluid ordering in He mixtures [1]. The most general Hamiltonian of the model is given by

$$H_I = -J \sum_{\langle ij \rangle} S_i S_j - K \sum_{\langle ij \rangle} S_i^2 S_j^2 + L \sum_{\langle ij \rangle} (S_i^2 S_j + S_i S_j^2) + D \sum_i S_i^2 + H \sum_i S_i \quad (1)$$

which is equivalent to the lattice gas Hamiltonian under some transformations [2] – [4]. $\langle ij \rangle$ denotes summation over all nearest-neighbor (nn) pairs of sites and $s_i = -1, 0, 1$. The parameters J , K , L , D and H are bilinear, biquadratic, dipole-quadrupole interaction terms, the single-ion anisotropy constant and the external field term. The versions of the model have been applied to the physical systems such as the solid-liquid-gas systems [5], the multicomponent fluids [6], the microemulsions [7], the semiconductor alloys

[8] – [10], He³-He⁴ mixtures [1, 11], the binary alloys [12] and the magnetic spin systems [13] – [16].

The spin-1 Ising model with dipole-quadrupole interaction was firstly studied using molecular field approximation [6, 17, 18] and the transfer matrix method [19] to investigate the tricritical and multicritical points for selected values of the ℓ parameter on one and two dimension. The spin-1 Ising model has also applied to two dimensional ternary graphite intercalation compounds (GIC's) for investigating the influence of the dipole-quadrupole interaction on the melting point using Monte Carlo method [20]. The model has been used for estimating the critical concentration value of the (GaAs)_{1-x}Ge_{2x} alloy by Kikuchi approximation [9, 10] and Cluster variation method [21, 22]. These studies show that the dipol-quadrupol interaction term is very effective on the critical concentration value of the (III – V)_{1-x}IV_x ternary alloys [23] and it can be dominant on the phase space [18, 19, 24]. However, the infinite lattice critical behaviors of the order parameter (M) and the susceptibility (χ) with the dipol-quadrupol interaction ($\ell = L/J$) has not been studied yet. In our previous paper [25], it was shown that the dipol-quadrupol interaction (ℓ) prevents the one of the spin species ($S = +1$ or -1) on the BEG model ($J \neq 0$, $K \neq 0$, $D \neq 0$) and breaks the symmetry in the Hamiltonian

similar to the external magnetic field (h) [26]. As a result of this, the dense ferromagnetic ($df(+)$, $df(-)$) and ferromagnetic ($F(+)$, $F(-)$) phases occur on the ground state phase diagram for nonzero ℓ value. Furthermore, model exhibits the reentrant, successive and multi phase transitions in the interval $-0.15 \leq \ell \leq 0.15$ and it does not show any phase transition at the large ℓ value ($\ell > 0.15$).

The aim of this study is to investigate the critical behavior of the BEG model with the dipol-quadrupol interaction (ℓ) and to estimate the power laws and the finite size scaling relations for the order parameter (M) and the susceptibility (χ) in the $\ell = L/J > 0$ region. In order to expose the effects of the dipol-quadrupol interaction ($\ell = L/J$), the biquadratic interaction ($k = K/J$), the single-ion anisotropy term and the external magnetic field ($h = H/J$) have been taken zero ($d = 0$, $k = 0$ and $h = 0$). These terms were studied in our previous papers and the effects of them on the phase space and the critical behavior of the BEG model were discussed [25] – [29].

The temperature dependence of the order parameters (M , Q), the susceptibility (χ), the specific heat (C/k) and the Ising energy (H_I) have been computed on the fcc lattice with linear dimension $L = 4, 6, 8, 9$ and 12 . The finite lattice critical temperatures are estimated from the maxima of the

susceptibility (χ) for the fcc lattice with periodic boundary conditions. In order to expose the influence of the dipole-quadrupole interaction, the thermodynamic quantities have been calculated using CA heating [25], [27] – [29] algorithm on the fcc lattice for $L= 4, 6, 8, 9$ and 12 (The total number of sites is $N = 4L^3$) with the periodic boundary conditions. The fcc lattice can be built from four interpenetrating simple cubic lattices. The linear dimension $L= 12$ of face centered cubic lattice corresponds to the $L= 20$ in simple cubic lattice. Hence, the data are analyzed within the framework of the finite-size scaling theory for the BEG model with the dipol-quadrupol interaction (ℓ).

The Creutz cellular automaton (CCA) is faster than the conventional Monte Carlo method (MC) [31]. The CCA does not need high quality random numbers and it is a new and an alternative simulation method for physical systems [25] – [29], [30] – [33]. Furthermore, the results obtained using CA algorithm and its improved versions are in good agreement with the universal critical behavior for the BEG model. Thus the simulations have been carried out using a cellular automaton heating algorithm which successfully produces the critical behavior of the Ising model [25], [27] – [29]. During the heating cycle, energy is added to the spin system through the second variables (H_K) after the 2.000.000 cellular automaton steps. The heating rate is equal to

$0.08H_K$ per site. The computed values of the thermodynamic quantities are averages over the lattice and the number of time steps (2.000.000) with discard of the first 100.000 time steps during the cellular automaton develops.

For the finite size lattice, the order parameters M and Q are given by

$$M = \frac{1}{L^3} \sum_i S_i \quad (2)$$

$$Q = \frac{1}{L^3} \sum_i S_i^2 \quad (3)$$

The susceptibility and the specific heat are calculated with

$$\chi = L^3 \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT} \quad (4)$$

$$C = L^3 \frac{\langle H_I^2 \rangle - \langle H_I \rangle^2}{kT} \quad (5)$$

The expectation values in equation (5) and (6) are averages over the lattice and the number of the time steps.

In order to investigate the critical behavior of the BEG model with the dipole-quadrupole interaction, the thermodynamic quantities have been calculated using CA heating algorithm on the fcc lattice for $L= 4, 6, 8, 9$ and

12 (The total number of sites is $N = 4L^3$) with the periodic boundary conditions.

For the $d = 0$ and the $k = 0$ line, the model exhibits the second order Ferromagnetic-Paramagnetic phase transition [25] for $\ell = 0$ while the susceptibility (χ) have a characteristic peak. With the increasing ℓ value in the interval $0 \leq \ell = L/J \leq 0.01$, the characteristic peak of susceptibility occurs at the higher critical temperature and its peak value decreases. The effect of the ℓ parameter is similar to those coming from the external magnetic magnetic field [25, 26, 33].

At $T = T_C(L)$, the order parameter values ($M(T_C(L), \ell)$) have been estimated for the increasing ℓ value in the interval $0 \leq \ell = L/J \leq 0.01$ on the different lattice sizes $L = 4, 6, 8, 9$ and 12 and illustrated in figure (1a). The results show that there is a considerable finite size effect near the $\ell = 0$. The $M(T_C(L), \ell)$ tends to zero with the increasing lattice sizes at $\ell = 0$. However the $M(T_C(L), \ell)$ goes to the constant value (~ 0.5) for all lattice size with the increasing value of ℓ . The susceptibility data $\chi(T_C(L), \ell)$ are plotted in figure (1b) for ℓ values in the interval $0 \leq \ell \leq 0.01$ on the different lattice sizes $L = 4, 6, 8, 9$ and 12 . Figure (1b) obviously shows that the susceptibility data $\chi(T_C(L), \ell)$ tend to infinity with increasing lattice size at

$\ell = 0$. Around the $\ell = 0$ value, the data show the dependence on the lattice size and $\chi(T_C(L), \ell)$ is a decreasing function of ℓ for the all lattice size.

The dipol-quadrupol interaction on the spin system shows a similar effect with the external magnetic field. As it is seen in figure (1), the order parameter (M) and the susceptibility (χ) are the functions of ℓ . For the determination of power-law exponent δ_ℓ , the power law relations of the thermodynamic functions (M and χ) for the dipol-quadrupol interaction (ℓ) have been considered as similar expressions to the power-laws of external magnetic field (h) [26, 34]. Therefore, the power laws of the order parameter (M) and the susceptibility (χ) at $T = T_C$ have been described by

$$M(T_C, \ell) = B_\ell |\ell|^{1/\delta_\ell} \quad (6)$$

$$\chi(T_C, \ell) = C_\ell |\ell|^{(1-\delta_\ell)/\delta_\ell} \quad (7)$$

where B_ℓ and C_ℓ are the order parameter and the susceptibility amplitudes. In the interval $0 \leq \ell \leq 0.01$, the order parameter (M), the critical exponent $\delta_\ell(L)$ and the order parameter amplitude $B_\ell(L)$ on each lattice size (L) are obtained from the best fit to straight lines in the Log-Log plot of the data (Figure (2a)). The estimated $\delta_\ell(L)$ and $B_\ell(L)$ values are plotted against

$L^{-1/\nu}$ in figure (2b) and (c). The extrapolations ($L^{-1/\nu} \rightarrow 0$) of data which lie on straight lines give the infinite lattice values as $1/\delta_\ell(\infty) = 0.193 \pm 0.005$ and $B_\ell(\infty) = 0.98 \pm 0.06$. The value $\delta_\ell = 5.18$ is in good agreement with universal value ($\delta_h = 5$) for external magnetic field [26, 34].

In figure 3, the critical exponent $\delta_\ell(L)$ and the susceptibility amplitude $C_\ell(L)$ are obtained from the susceptibility data ($\chi(T_C(L), \ell)$). The Log-Log plot of $\chi(T_C(L), \ell)$ against ℓ in the interval $0 \leq \ell \leq 0.001$ yields $(1 - \delta_L(L))/\delta_L(L)$ and $C_\ell(L)$ in figure (3a). The extrapolation of these quantities gives $(1 - \delta_\ell(\infty))/\delta_\ell(\infty) = -0.80 \pm 0.05$ and $C_\ell(\infty) = 0.008 \pm 0.001$ (Figure (3b) and 3(c)). Therefore, the value of $\delta_\ell(\infty)$ is obtained as 5 which is equal to the universal value $\delta_h = 5$ for the external magnetic field.

The finite-size scaling relations [26] of the order parameter (M) and the susceptibility (χ) related to the dipol-quadrupol interaction ℓ can be defined by scaling relations related to the external magnetic field h as

$$M = L^{-\beta/\nu} X^o(L^{\delta_\ell \beta/\nu} |\ell|, L^{1/\nu} \varepsilon) \quad (8)$$

$$kT\chi = L^{\gamma/\nu} Y^o(L^{\gamma \delta_\ell / \nu (\delta_\ell - 1)} |\ell|, L^{1/\nu} \varepsilon) \quad (9)$$

with $\varepsilon = (T - T_C(\infty))/T_C(\infty)$ [26, 34].

At $T = T_C(\infty)$, the scaling functions X° and Y° are asymptotically reproduced as

$$X^\circ(x) = B_\ell x^{1/\delta_\ell} \quad (10)$$

$$Y^\circ(x) = C_\ell x^{(1-\delta_\ell)/\delta_\ell} \quad (11)$$

where $x = L^{\delta_\ell \beta / \nu} |\ell|$, B_ℓ and C_ℓ are the order parameter and the susceptibility amplitudes. The finite-size scaling plots of the order parameter data $M(T_C(\infty), \ell)$ at the infinite lattice critical temperature ($\varepsilon = 0$) are illustrated in figure 4. For $\delta_\ell = 5$, $\beta = 0.31$ and $\nu = 0.64$ universal values, the order parameter data lie on a single curve with the slope equal to $1/\delta_\ell = 0.2$ in the interval $0.229 \leq x \leq 2.875$. The estimated value is in good agreement with the value of the field critical exponent ($\delta_h=5$). Furthermore, the order parameter amplitude in equation (9) is estimated as $B_\ell = 1.096$. This value is in agreement with the linear extrapolation result (Figure. 2(c)). The finite-size scaling plots of the susceptibility data $\chi(T_C(\infty), \ell)$ are shown using $\delta_\ell = 5$, $\gamma = 1.25$ and $\nu = 0.64$ universal values in figure 5. As it is seen in figure 5, the scaling susceptibility data in the interval $0.236 \leq x \leq 3.018$ lie on a straight line with the slope $(1 - \delta_\ell)/\delta_\ell = -0.8$. It gives the value of the dipol-quadrupol critical exponent δ_ℓ as 5. The value of the straight line at

$\varkappa = 0$ gives the susceptibility amplitude as $C_\ell = 0.063$.

The previous studies implied that the dipol-quadrupol interaction ℓ on the spin-1 Ising model Hamiltonian is considered as a magnetic field-like perturbation [8, 35]. Our simulations exposed that the dipol-quadrupol interaction parameter ℓ has prevented the one of the spin species ($S = +1$ or -1) and it has broken the symmetry in the Hamiltonian. Really, the ℓ acts similar to the external magnetic field h over the spin system. However, the order parameter $M(T_C, \ell)$ and the susceptibility $\chi(T_C, \ell)$ behave according to the equations of state ($M \sim \ell^{1/\delta}$ and $\chi \sim \ell^{(1-\delta_\ell)/\delta_\ell}$) in the interval $0 \leq \ell = L/J \leq 0.01$ at the critical temperature. Moreover, the order parameter (M) and the susceptibility (χ) data are scaled well within the framework of the finite size scaling hypothesis (at $T_C(\infty)$ obtained for $\ell = 0$). The obtained value of the critical exponent δ_ℓ are in good agreement with the universal value ($\delta_h = 5$) of the external magnetic field. These results indicate that the dipol-quadrupol interaction parameter ℓ is similar to the external magnetic field h over the spin system. Therefore, ℓ can be considered as a magnetic field-like perturbation.

Acknowledgement

This work is supported by a grant from Gazi University (BAP:05/2003-07).

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Figure Captions

Figure.1. At $T = T_C(L)$ on the different lattice sizes $L = 4, 6, 8, 9$ and 12 in the interval $0 \leq \ell \leq 0.001$ for $d = 0$ and $k = 0$ (a) the order parameter values M against ℓ , the susceptibility values χ against ℓ .

Figure.2. On the different lattice sizes $L = 4, 6, 8, 9$ and 12 (a) Log-log plots of M versus ℓ , (b) The plot of $\delta_\ell(L)$ versus $L^{-1/\nu}$, (c) The plot of $B_\ell(L)$ versus $L^{-1/\nu}$.

Figure.3. On the different lattice sizes $L = 4, 6, 8, 9$ and 12 (a) Log-log plots of χ versus ℓ , (b) The plot of $\delta_\ell(L)$ versus $L^{-1/\nu}$, (c) The plot of $C_\ell(L)$ versus $L^{-1/\nu}$.

Figure.4. The finite-size scaling plot of the order parameter (M) for $T < T_C(\infty)$ on the different lattice sizes $L = 4, 6, 8, 9$ and 12

Figure 5. The finite-size scaling plot of the susceptibility (χ) for $T < T_C(\infty)$ on the different lattice sizes $L=4, 6, 8, 9$ and 12

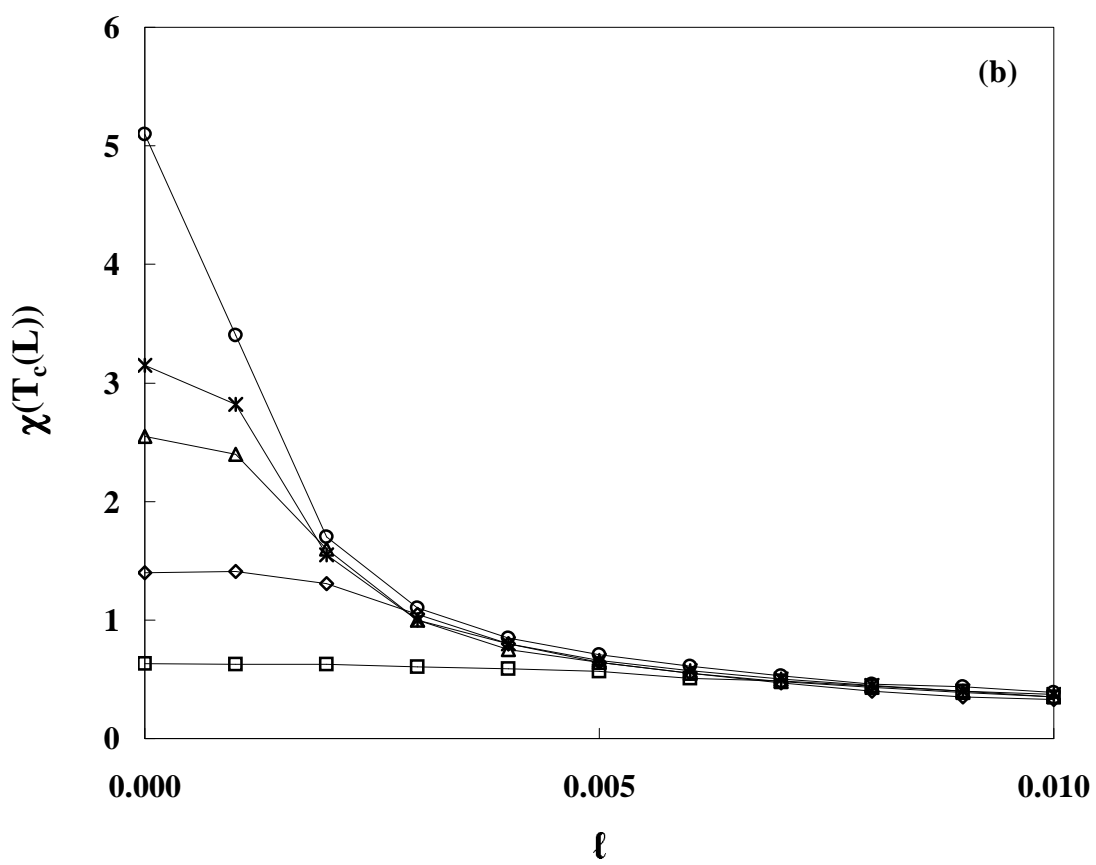
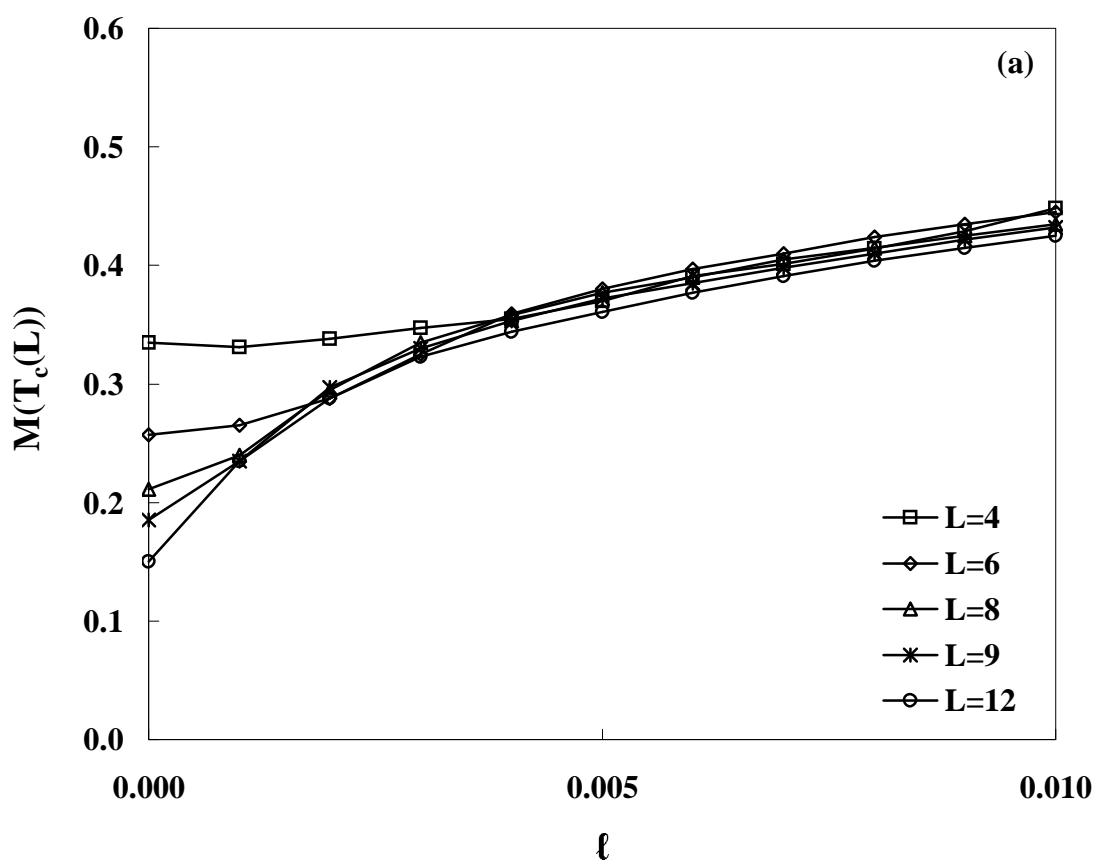


Fig.1

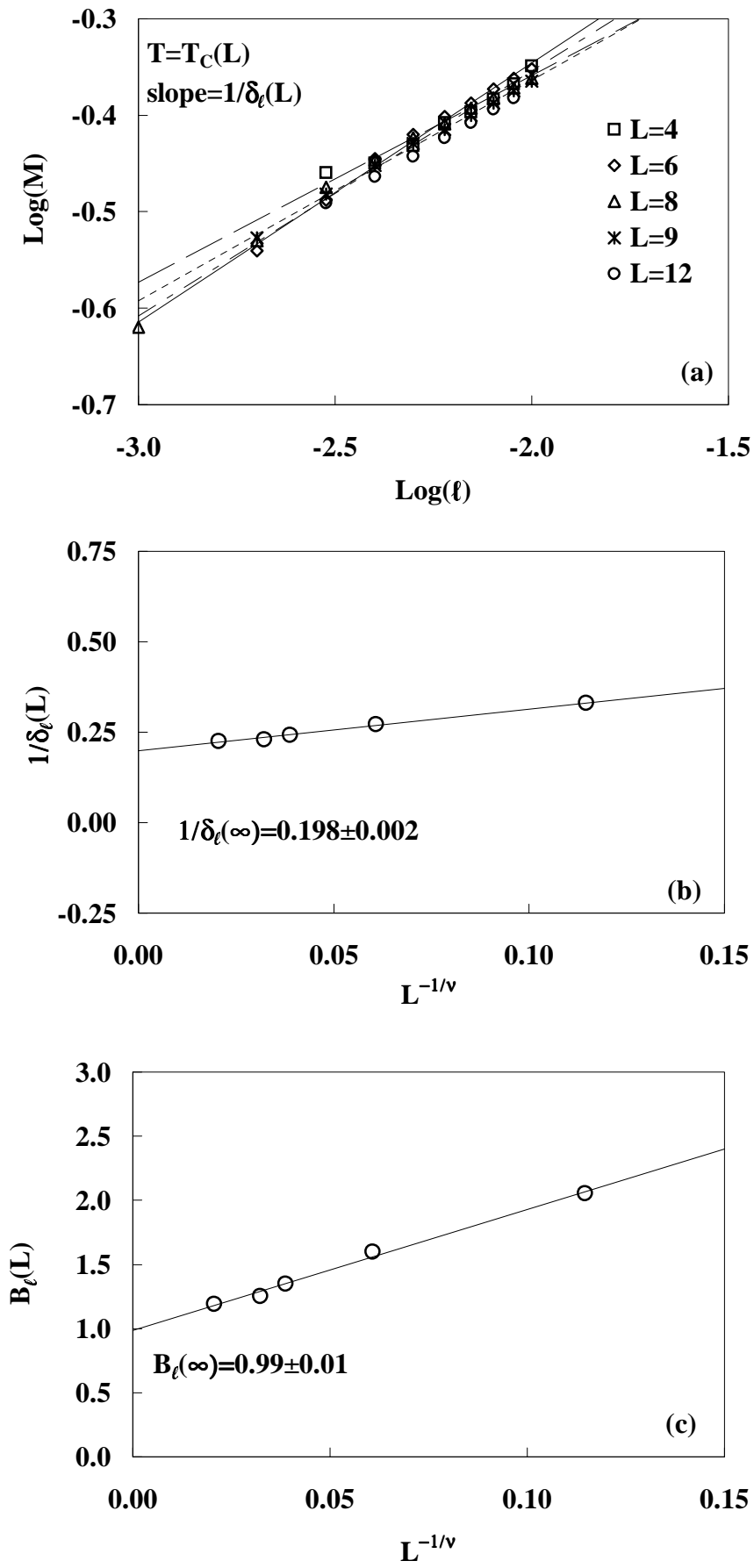


Fig. 2

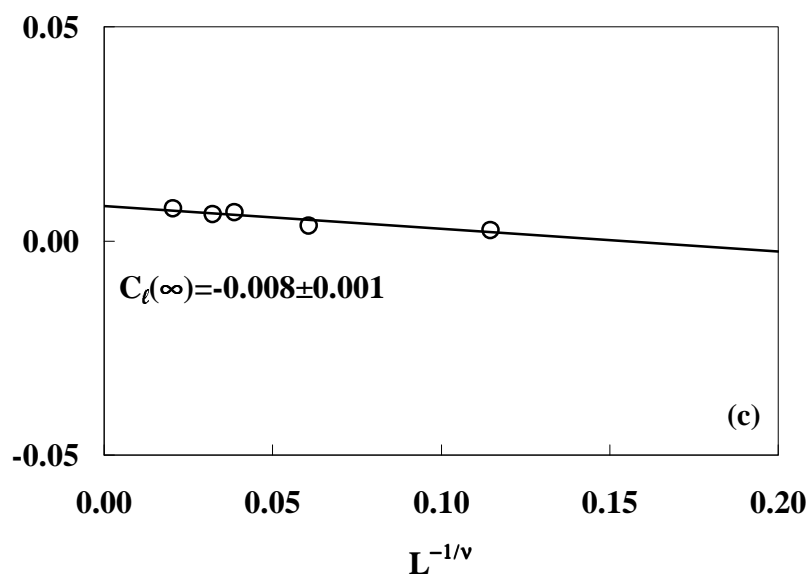
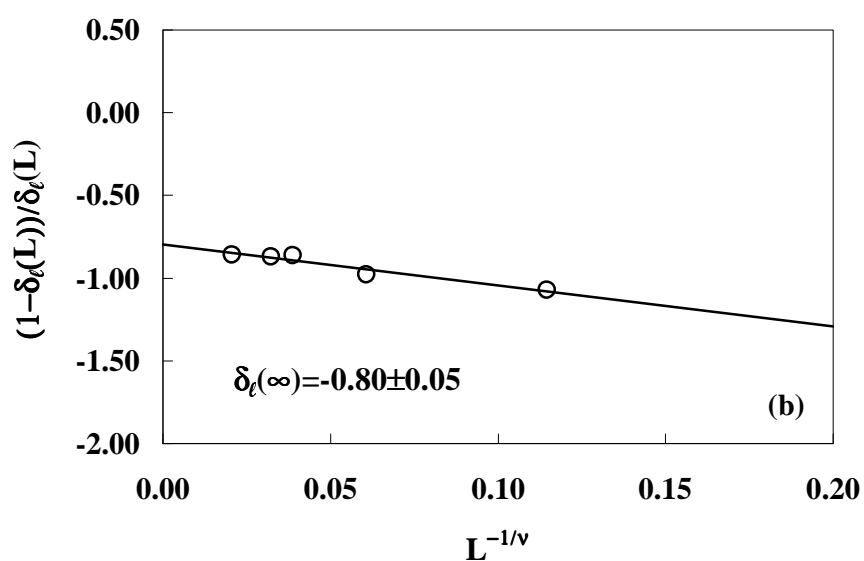
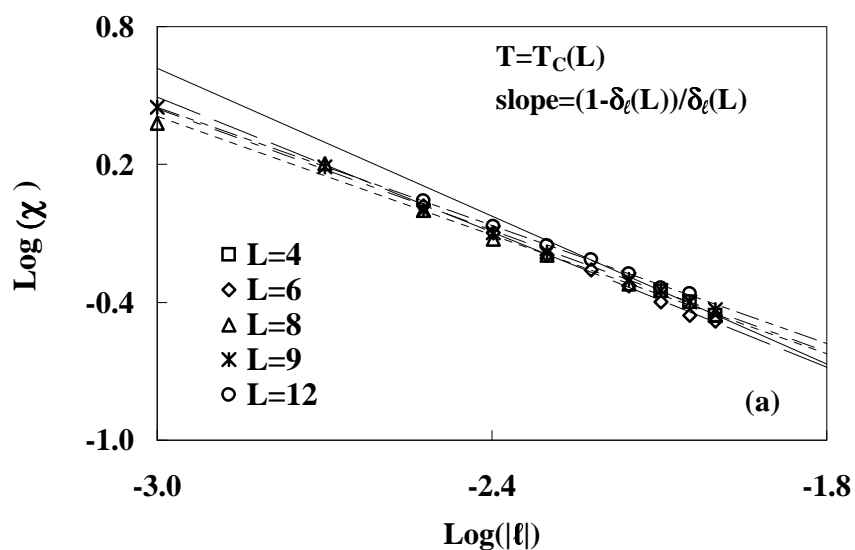


Fig. 3

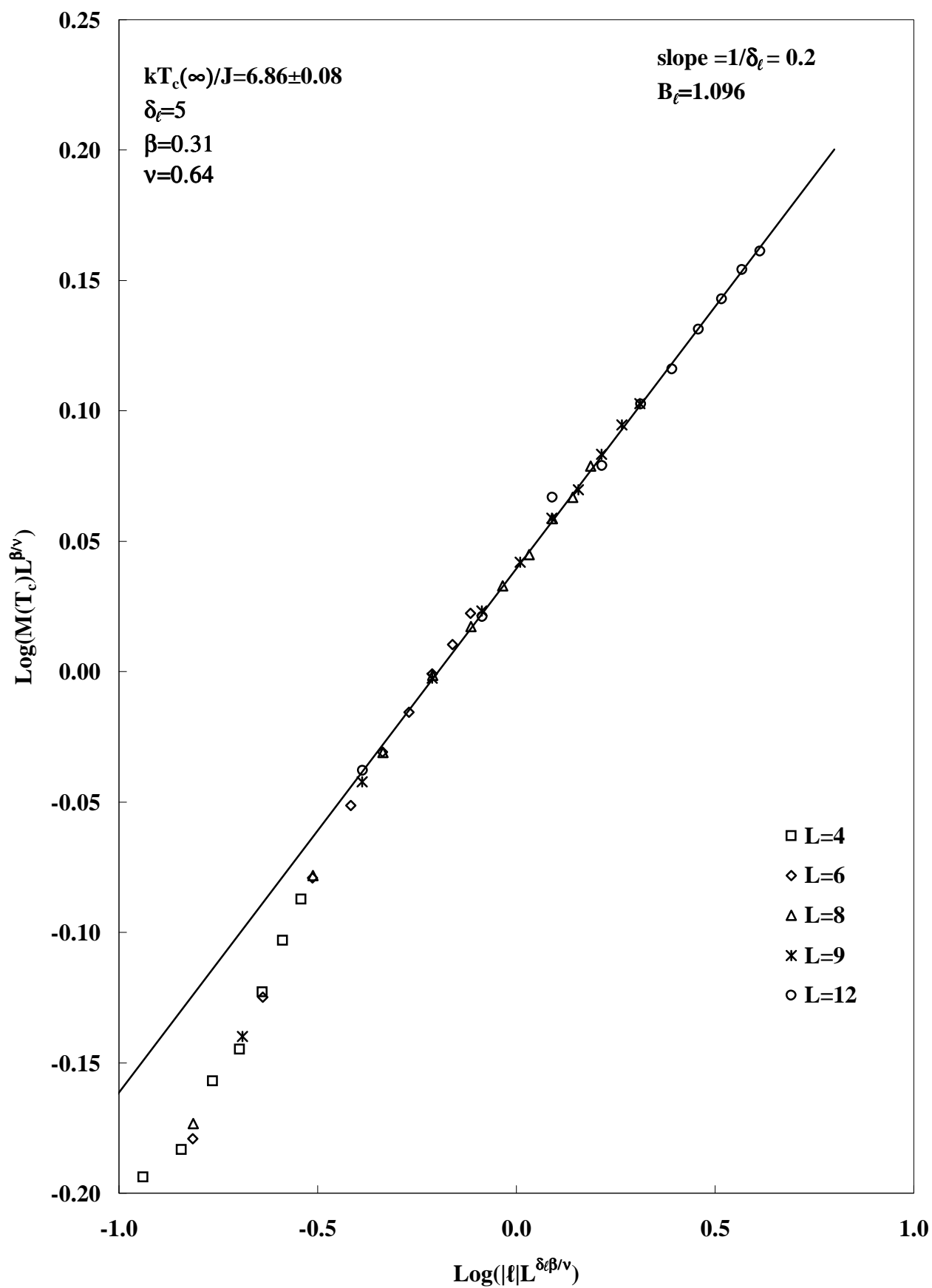


Fig.4

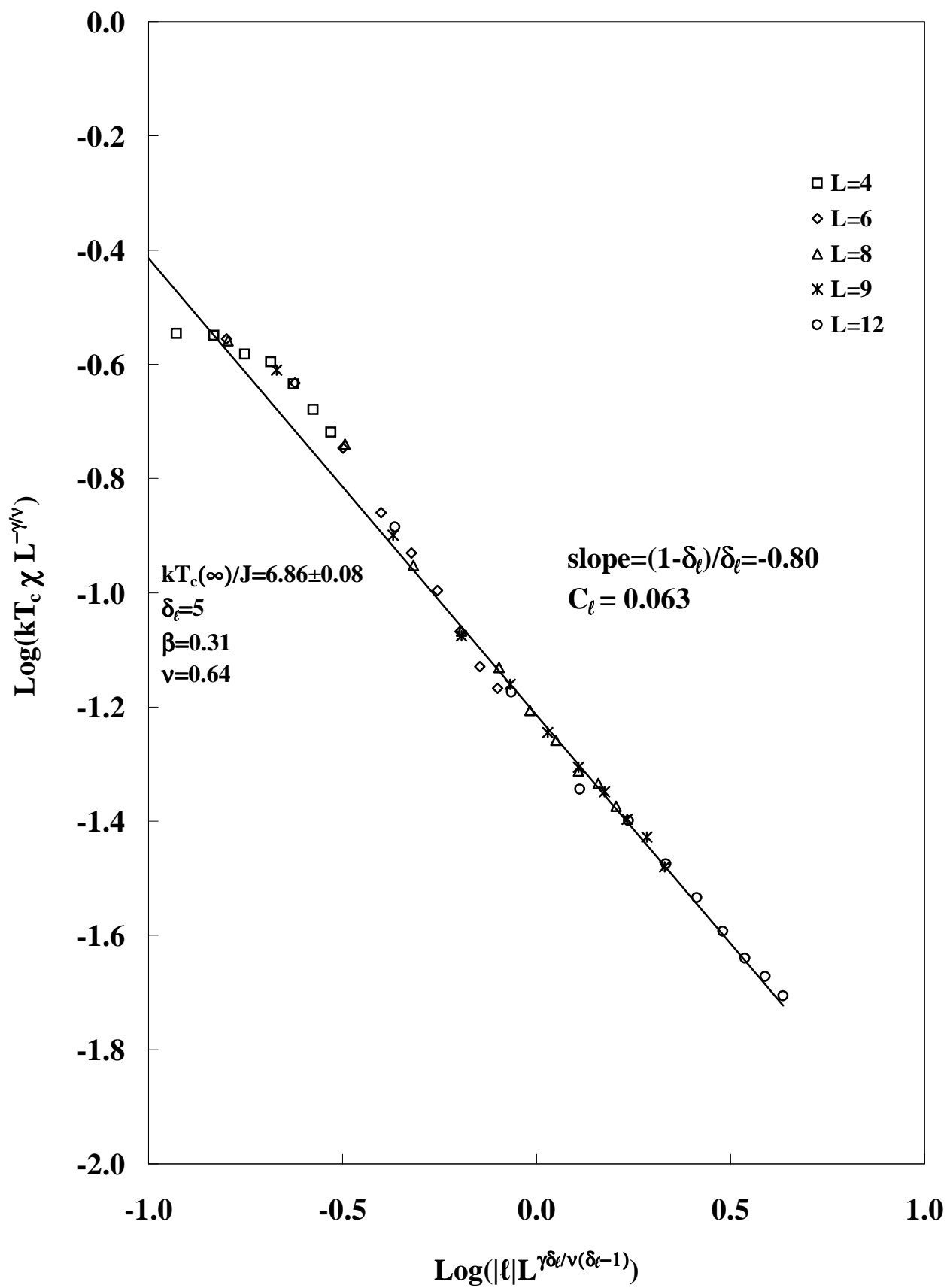


Fig.5